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* XPSIM, Vers. 1.06 *           *... extended Process Simulation ...*
* Cust/User "           " *           - INPUT -           * Job " " *
* Proj/Problem "           " *           * Date SEP 21, 2008 *

--- Simulation Input File ---
*-STMT-*
*XPSIM> ...generated by XpsimWin v.1.06 ...
*EXE-OPT> PAGELEN=66
*
100 RUN ID=PROB-07 USER=STAFF PROBLEM='MTBE SEPARATION'
200 DESC MTBE RECOVERY COLUMN
300 DESC APPLICATION TEST CASE
400 DIMENSION INPUT MET PRES=BAR
*
*
500 System Data
*
*
600 CHEMCOMP PRLN / C3 / IC4 / IBTE / BUT1 / 13BD / NC4 / BTT2 / BTC2 / +
    MEOH / IC5 / MTBE / TBA / TAME
700 THERMSET UID=SET1
800 METHODS AL=UNIFAC FV=IDEAL FL=IDEAL HS=IDEAL
*
*
900 Flowsheet Data
*
*
*
1000 COLUMN UID=C2
1100 PARA TRAY=32 CON REB NITER=20
1200 FEED STR=S1 TRAY=14
1300 DRAWOFF STR=S2 TRAY=0 PHASE=LIQ
1400 DRAWOFF STR=S3 TRAY=33 PHASE=LIQ RATE(VAR)=158.8
1500 PROFILE TRAY=0 LIQ=1100 TEMP=54.5 PRES=8 / TRAY=1 PRES=8.35 / TRAY=33 +
    TEMP=149 PRES=9.37
1600 HEAT TRAY=0 VAR
1700 HEAT TRAY=33 VAR
1800 SPEC RATE=0.998 RATIO STR=S3 REFSTR=S1 COMP=MTBE
1900 SPEC RATE=0.8 RATIO STR=LNET:1 REFSTR=S2
2000 PRINT TRACE=PART STREAM=1
*
2100 STREAM=S1 TEMP=71.1 PRES=10.35 RATE=1425.9 NORM XBASIS=M
2200 COMP PRLN:116.61 / C3:88.26 / IC4:978.17 / IBTE:8.75 / BUT1:343.78 / +
    13BD:6.02 / NC4:433.77 / BTT2:400.54 / BTC2:267.96 / MEOH:142.07 / +
    IC5:33.07 / MTBE:321.76 / TBA:0.55 / TAME:2.17
*
*
2300 END
--- End of Simulation Input File ---
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I) * PROBLEM GENERAL DATA *

- 1) * PROBLEM/PROJECT *
- 'MTBE RECOVERY COLUMN'
- 'APPLICATION TEST CASE'

- 2) * UNITS OF MEASURE *
- Input system METRIC - Output system METRIC

- INPUT AND OUTPUT UNITS -			
Time	- HR	Weight	- KG
Temperature	- CENT	Pressure	- BAR
Energy/Duty	- M-KCAL	Work	- KW
Liq volums	- CUMT	Vap Volume	- CUMT
Viscosity	- CP	Thermal cond	- KCAL/HMC
Surface tens	- DYCM	Std Vap Vol	- N-CUMT

Standard Vapor Volume is 23.64469 M3/KMOL
Reference Status - Temperature 15°C - Pressure 1 atm

Enthalpy is 0.0 for ideal gas at 298.15 K
Std entropy is for ideal gas at 298.15 K and 1 Atm

II) * DEFINED COMPONENTS *

* No of Chemical Components 14
No of Hypothetical/Petroleum Components 0

No	1	2	3	4	5
CAS Registry no.	115-07-1	74-98-6	75-28-5	115-11-7	106-98-9
Name	PROPENE	PROPANE	ISOBUTANE	ISOBUTENE	1-BUTENE
Component Key	PRLN	C3	IC4	IBTE	BUT1
Type	LIBRARY	LIBRARY	LIBRARY	LIBRARY	LIBRARY
Class	UHYD	SHYD	SHYD	UHYD	UHYD
Formula	C3H6	C3H8	C4H10	C4H8	C4H8
Molecular weight	42.080	44.100	58.120	56.107	56.107
Boiling point,CENT	-47.69	-42.10	-11.73	-6.95	-6.26
Std spec. gravity	0.51987	0.50430	0.55891	0.59848	0.59728
Critical temp,CENT	91.70	96.67	134.99	144.75	146.42
Critical pres,BAR	46.010	42.490	36.480	39.980	40.230
Critical vol,CUMT	0.180602	0.203227	0.262988	0.238755	0.239775
Critical Z	0.273935	0.280844	0.282728	0.274732	0.276526
Acentric factor	0.144000	0.153000	0.183000	0.194000	0.192000
Lat. heat, KC/KMOL	4369.846	4501.865	5046.152	5185.873	5096.479
H form, KC/KMOL	5608.232	-24805.360	-32149.941	-4033.663	-26.802
G form, KC/KMOL	-16232.370	-44046.738	-53185.852	-24941.393	-21789.071
Std entr, KC/KML-C	73.25374	64.53590	70.55479	70.12487	72.99101
No	6	7	8	9	10
CAS Registry no.	106-99-0	106-97-8	590-18-1	624-64-6	67-56-1
Name	1,3-BUTADIENE	BUTANE	TRANS-2-BUTENE	CIS-2-BUTENE	METHANOL
Component Key	13BD	NC4	BTT2	BTC2	MEOH
Type	LIBRARY	LIBRARY	LIBRARY	LIBRARY	LIBRARY
Class	UHYD	SHYD	UHYD	UHYD	ALCO
Formula	C4H6	C4H10	C4H8	C4H8	CH4O
Molecular weight	54.090	58.120	56.108	56.108	32.040
Boiling point,CENT	-4.47	-0.50	0.88	3.71	64.54
Std spec. gravity	0.62654	0.58434	0.60972	0.62972	0.79508
Critical temp,CENT	152.00	152.03	155.48	162.43	239.49
Critical pres,BAR	43.300	37.980	39.847	41.967	80.920
Critical vol,CUMT	0.220777	0.254914	0.238002	0.234002	0.117795
Critical Z	0.270450	0.273882	0.266124	0.271174	0.223644
Acentric factor	0.194000	0.200000	0.205000	0.201000	0.564000
Lat. heat, KC/KMOL	5336.884	5249.344	5421.998	5575.045	8575.612
H form, KC/KMOL	26316.252	-30039.928	-2669.989	-1669.993	-48004.709
G form, KC/KMOL	6469.575	-52101.286	-23796.810	-23106.892	-65074.133
Std entr, KC/KML-C	66.56608	73.99416	70.85971	71.89971	57.25113
No	11	12	13	14	
CAS Registry no.	78-78-4	1634-04-4	75-65-0	994-05-8	
Name	ISOPENTANE	METHYL TERTBUTYL ETH	TERT-BUTYL ALCOHOL	TERT-AMYL ETHER	
Component Key	IC5	MTBE	TBA	TAME	
Type	LIBRARY	LIBRARY	LIBRARY	LIBRARY	
Class	SHYD	ETHE	ALCO	ETHE	
Formula	C5H12	C5H12O	C4H10O	C6H14O	
Molecular weight	72.150	88.149	74.122	102.177	
Boiling point,CENT	27.88	55.15	82.34	86.10	
Std spec. gravity	0.62469	0.74541	0.79166	0.77447	
Critical temp,CENT	187.28	223.95	233.06	258.05	
Critical pres,BAR	33.830	34.300	39.730	32.500	
Critical vol,CUMT	0.305722	0.313700	0.274528	0.376002	
Critical Z	0.270180	0.260346	0.259156	0.276696	
Acentric factor	0.227000	0.267000	0.613000	0.346268	
Lat. heat, KC/KMOL	5806.159	6602.998	9558.912	7.505	
H form, KC/KMOL	-36895.129	-69983.322	-74638.665	-75579.609	
G form, KC/KMOL	-61363.439	-98816.905	-97875.015	-107237.051	
Std entr, KC/KML-C	82.06712	96.70831	77.93510	106.17958	

III) * PVT/THERMO/TRANSPORT PROPERTIES CALCULATION METHODS *

* CALCULATION SET 1 - SET1 *

ACTIVITY coefficient	UNIFAC	- UNIFAC ACTIVITY
FUGACITY - Vapor	IDEAL	- IDEAL/LIBRARY
FUGACITY - Liquid	IDEAL	- IDEAL/LIBRARY
ENTHALPY - Vapor	IDEAL	- IDEAL/LIBRARY
ENTHALPY - Liquid	IDEAL	- IDEAL/LIBRARY
ENTROPY - Vapor	IDEAL	- IDEAL/LIBRARY
ENTROPY - Liquid	IDEAL	- IDEAL/LIBRARY

- LIMITS AND OPTIONS -

Temperature - Min	-223.15 CENT	- Max	1200.05 CENT
Pressure - Min	0.980667E-05 BAR	- Max	2942.00 BAR

Lowest significant composition 0.10000000E-19

Water K-values are calculated based on
'Vapor Pressure curve',
Water thermo-props are calculated based on
'Saturated conditions',
Water solubility in hydr phases calculated based on
'API solubility in HC mixtures'

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* XPSIM, Vers. 1.06 *
* Cust/User "STAFF" *
* Proj/Problem "MTBE SEPARATION" *
* Date SEP 21, 2008 *
* Job "PROB-07" *
* Page 0005 *
*... extended Process Simulation ...*
- INPUT -
- UNIT 1 - C2 -

*** UNIT 1 - 'C2' - 'DISTILLATION COLUMN' ***
--- Feed Streams ---
'S1'
- Product Streams -
'S2'
'S3'

1) * PARAMETERS *

No of theoretical trays 32
- condenser
- reboiler

No of Feeds 1
Products 2
Heater-Coolers 2
Pump-Arounds 0
Specifications 2

Calculation method 'SURE'
Maximum no of iterations 20
Max no of iterations with no error improvements 3

2) * CALCULATION TOLERANCES *
Bubble point 0.001000 Enthalpy balances 0.001000
Component balances 0.001000 Composition sums 0.001000

3) * COLUMN FEEDS *

1 - Stream S1 ON tray 14 - Flowrate FIXED - Temperature FIXED

4) * PRODUCT STREAMS *

1 - Stream S2 extracted as LIQUID from condenser - Flowrate NOT GIVEN
Material balance closed on this stream

2 - Stream S3 extracted as LIQUID from reboiler - Flowrate VARIABLE
Initial flowrate 158.800 KMOL/HR

5) * HEATER / COOLERS *

1 - CONDENSER - User Id 0
Duty is VARIABLE - Initial value 0.000 M-KCAL /HR

2 - REBOILER - User Id 33
Duty is VARIABLE - Initial value 0.000 M-KCAL /HR

6) * CONDENSER/REBOILER SPECS *
Reboiler is a KETTLE type
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7) * INITIAL TEMPERATURE/FLOW-RATE ESTIMATES *

*** TRAY ***		OUTLET * LIQUID RATE * KMOL/HR	* TEMPERATURE * CENT	* PRESSURE * BAR
CON		1100.000	54.500	8.0000
1		NOT GIVEN	NOT GIVEN	8.3500
REB		NOT GIVEN	149.000	9.3700

8) * PERFORMANCE SPECIFICATIONS *

Spec 1
* Hold sum od partial MOLAR flow-rates of component(s)
12) METHYL TERTBUTYL ETH
contained in stream(s)
'S3 '- LIQUID DRAW-OFF FROM REBOILER
DIVIDED BY sum of partial MOLAR flow-rate of same component(s)
contained in streams
'S1 '- FEED 1 ON TRAY 14
at EQUAL TO 0.998000
Tolerance (RELATIVE) 0.010000

Spec 2
* Hold MOLAR flow-rate of stream
- NET LIQUID INLET TO TRAY 1
DIVIDED BY sum of MOLAR flow-rates of streams
'S2 '- LIQUID DRAW-OFF FROM CONDENSER
at EQUAL TO 0.800000
Tolerance (RELATIVE) 0.010000

*** STREAM 'S1' ***							
- Temperature		71.100 CENT		- Pressure		10.3500 BAR	
				----- GLOBAL STREAM -----			
* No	* Component	*	- Mols	- Mol fr-	- weight	- Wt fr-	
1	PROPENE		52.895	0.037096	2225.819	0.026663	
2	PROPANE		40.035	0.028077	1765.554	0.021149	
3	ISOBUTANE		443.703	0.311174	25788.036	0.308911	
4	ISOBUTENE		3.969	0.002784	222.691	0.002668	
5	1-BUTENE		155.941	0.109363	8749.354	0.104807	
6	1,3-BUTADIENE		2.731	0.001915	147.704	0.001769	
7	BUTANE		196.760	0.137990	11435.718	0.136987	
8	TRANS-2-BUTENE		181.687	0.127419	10194.104	0.122114	
9	CIS-2-BUTENE		121.548	0.085243	6819.824	0.081694	
10	METHANOL		64.444	0.045195	2064.777	0.024734	
11	ISOPENTANE		15.001	0.010520	1082.303	0.012965	
12	METHYL TERTBUTYL ETH		145.952	0.102358	12865.534	0.154114	
13	TERT-BUTYL ALCOHOL		0.249	0.000175	18.492	0.000222	
14	TERT-AMYL ETHER		0.984	0.000690	100.575	0.001205	

* TOTAL *			1425.900	1.000000	83480.486	1.000000	
			KMOL		KG		

V) **** STREAM / UNITS DICTIONARY ****

1) STREAMS-UNITS CROSS-REFERENCE TABLE				
No	Stream Id	Description/Service	Product of Unit	Feed of Unit(s)
1	S1			1 C2
2	S2		1 C2	
3	S3		1 C2	

2) UNITS-STREAMS CROSS-REFERENCE TABLE				
No	Unit	Unit Description	Feed Streams	Product Streams
1	C2		1 S1	2 S2 3 S3

VI) **** RUN STATISTICS ****

* No of streams	3
process operations	1
topping structures	0
control operations	0
set operations	0

The calculation is NOT a RECYCLE PROBLEM
Calculation sequence defined by input sequence

*** SIMULATION TRACE FOLLOWS ***

... New/output binary file 'PROB-07 ' initialized ...

. Stream 'S1 ' flashed .

. Feed/Recycle streams processed .

Intermediate column calculation printout

... Feed S1 on tray 14 flashed at 8.7644 BAR ...

- Temp 64.71 CENT, Rate, Liquid 1352.673 KMOL, Vapor 73.227 KMOL

- at iter 0, err sum 22.9373 , max err sum 1.51082 - adj. factor 0.000000

DK/K - max .15578E-02 - min .82117E-09 - avg 0.000119

Error sums, total 22.9373 , BP 7.18414 , H 0.861477 , Comp 14.8917

- Maximum Relative Errors -

* BP 0.557243 at tray 14 * H -0.163942 at tray 14

Tray Glob Mat Bal -0.789632 at tray 19 * Tray Part Mat Bal 0.253113 for comp 14 at tray 14

Coln Part Mat Bal 0.398452 for comp 14

*** INITIAL COLUMN STATUS ***			***		
* TRAY *	TEMP	** -TOTAL LIQ &	VAP OUTLET-	* - LIQ. & VAP. DRAW-OFF -	* BP.ERROR * ENT.BAL.ERR.*
0	54.500	1520.520	0.000	1267.100 0.000	-0.059260 0.000000
1	57.364	253.420	1520.520	0.000 0.000	-0.223366 0.073621
2	60.227	253.420	1520.520	0.000 0.000	-0.253496 0.058535
3	63.091	253.420	1520.520	0.000 0.000	-0.269359 0.050839
4	65.955	253.420	1520.520	0.000 0.000	-0.270812 0.042531
5	68.818	253.420	1520.520	0.000 0.000	-0.253887 0.034749
6	71.682	253.420	1520.520	0.000 0.000	-0.216594 0.028212
7	74.545	253.420	1520.520	0.000 0.000	-0.158566 0.023057
8	77.409	253.420	1520.520	0.000 0.000	-0.080773 0.019288
9	80.273	253.420	1520.520	0.000 0.000	0.014138 0.016925
10	83.136	253.420	1520.520	0.000 0.000	0.121587 0.015952
11	86.000	253.420	1520.520	0.000 0.000	0.235666 0.016193
12	88.864	253.420	1520.520	0.000 0.000	0.350671 0.017234
13	91.727	253.420	1520.520	0.000 0.000	0.462070 0.000228
14	94.591	1606.093	1447.293	0.000 0.000	0.557243 -0.163942
15	97.455	1606.093	1447.293	0.000 0.000	0.418871 0.030378
16	100.318	1606.093	1447.293	0.000 0.000	0.257950 0.041317
17	103.182	1606.093	1447.293	0.000 0.000	0.081891 0.044543
18	106.045	1606.093	1447.293	0.000 0.000	-0.077660 0.040646
19	108.909	1606.093	1447.293	0.000 0.000	-0.195295 0.030813
20	111.773	1606.093	1447.293	0.000 0.000	-0.267523 0.019711
21	114.636	1606.093	1447.293	0.000 0.000	-0.304151 0.010541
22	117.500	1606.093	1447.293	0.000 0.000	-0.315932 0.003873
23	120.364	1606.093	1447.293	0.000 0.000	-0.310208 -0.000832
24	123.227	1606.093	1447.293	0.000 0.000	-0.291755 -0.004108
25	126.091	1606.093	1447.293	0.000 0.000	-0.264150 -0.006310
26	128.955	1606.093	1447.293	0.000 0.000	-0.230191 -0.007720
27	131.818	1606.093	1447.293	0.000 0.000	-0.191889 -0.008591
28	134.682	1606.093	1447.293	0.000 0.000	-0.150533 -0.009139
29	137.545	1606.093	1447.293	0.000 0.000	-0.106883 -0.009538
30	140.409	1606.093	1447.293	0.000 0.000	-0.061393 -0.009944
31	143.273	1606.093	1447.293	0.000 0.000	-0.014392 -0.010540
32	146.136	1606.093	1447.293	0.000 0.000	0.033728 -0.011630
33	149.000	158.800	1447.293	158.800 0.000	0.082257 0.000000

* HEATERS / COOLERS *

TRAY 0 - DUTY -7435.074 M-KCAL

TRAY 33 - DUTY 8158.323 M-KCAL

* SPECIFICATIONS *		GIVEN VALUE		CALC VALUE		ERROR CONV	
NO	TYPE						
1	RECOVERY RAT		0.998000		1.077554	0.038348	N
2	RATE RAT		0.800000		0.200000	-0.693147	N

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* Cust/User "STAFF"                               " *                               *
* Proj/Problem "MTBE SEPARATION"                   " *                               *
* Date SEP 21, 2008 *                               * Job "PROB-07" " *

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- at iter 1, err sum 16.8735, max err sum 1.16083 - adj. factor 0.259619
DK/K - max .17677E-02 - min .54836E-09 - avg 0.000127
DT max - abs 22.4442 - rel 0.031260 DR max - abs 244.5478 - rel 0.285714
Error sums, total 16.8735, BP 5.04828, H 0.695564, Comp 11.1297
- Maximum Relative Errors -
* BP 0.403158 at tray 14 * H -0.080564 at tray 13
Tray Glob Mat Bal -0.677104 at tray 19 * Tray Part Mat Bal 0.224108 for comp 14 at tray 14
Coln Part Mat Bal 0.223950 for comp 14

- at iter 2, err sum 14.6883, max err sum 1.03605 - adj. factor 0.112667
DK/K - max .12673E-02 - min .30232E-10 - avg 0.000090
DT max - abs 30.0000 - rel 0.041479 DR max - abs 190.1778 - rel 0.127464
Error sums, total 14.6883, BP 4.14357, H 0.609411, Comp 9.93533
- Maximum Relative Errors -
* BP 0.351602 at tray 14 * H -0.072786 at tray 13
Tray Glob Mat Bal -0.611661 at tray 20 * Tray Part Mat Bal 0.204908 for comp 14 at tray 14
Coln Part Mat Bal 0.187733 for comp 14

- at iter 3, err sum 10.5135, max err sum 0.756323 - adj. factor 0.304890
DK/K - max .18457E-02 - min .91591E-10 - avg 0.000142
DT max - abs 30.0000 - rel 0.040904 DR max - abs 320.4964 - rel 0.237178
Error sums, total 10.5135, BP 2.79947, H 0.425982, Comp 7.28806
- Maximum Relative Errors -
* BP 0.222967 at tray 13 * H -0.050211 at tray 13
Tray Glob Mat Bal -0.483145 at tray 20 * Tray Part Mat Bal 0.143316 for comp 14 at tray 14
Coln Part Mat Bal 0.118822 for comp 14

- at iter 4, err sum 5.92861, max err sum 0.409339 - adj. factor 0.534829
DK/K - max .14724E-02 - min .66939E-10 - avg 0.000107
DT max - abs 23.4926 - rel 0.032234 DR max - abs 445.3800 - rel 0.285714
Error sums, total 5.92861, BP 1.55278, H 0.273707, Comp 4.10212
- Maximum Relative Errors -
* BP 0.100894 at tray 11 * H 0.034215 at tray 6
Tray Glob Mat Bal -0.274230 at tray 20 * Tray Part Mat Bal 0.046583 for comp 14 at tray 14
Coln Part Mat Bal 0.061189 for comp 14

- at iter 5, err sum 1.34751, max err sum 0.122064 - adj. factor 0.873144
DK/K - max .94503E-03 - min .23186E-11 - avg 0.000066
DT max - abs 15.3350 - rel 0.021703 DR max - abs 558.0796 - rel 0.285714
Error sums, total 1.34751, BP 0.348674, H 0.132995, Comp 0.865841
- Maximum Relative Errors -
* BP -0.034167 at tray 4 * H 0.032451 at tray 7
Tray Glob Mat Bal 0.055445 at tray 4 * Tray Part Mat Bal 0.011652 for comp 12 at tray 4
Coln Part Mat Bal 0.016179 for comp 14

- at iter 6, err sum 0.366166, max err sum 0.615095E-01 - adj. factor 1.000000
DK/K - max .15175E-02 - min .35591E-10 - avg 0.000121
DT max - abs 5.2445 - rel 0.008334 DR max - abs 306.8152 - rel 0.146221
Error sums, total 0.366166, BP 0.107726, H 0.212935E-01, Comp 0.237146
- Maximum Relative Errors -
* BP -0.021760 at tray 6 * H 0.005193 at tray 7
Tray Glob Mat Bal 0.034556 at tray 6 * Tray Part Mat Bal 0.006678 for comp 12 at tray 6
Coln Part Mat Bal 0.003349 for comp 14

- at iter 7, err sum 0.335314, max err sum 0.621483E-01 - adj. factor 1.000000
DK/K - max .75925E-03 - min .33910E-10 - avg 0.000067
DT max - abs 3.8665 - rel 0.006603 DR max - abs 74.0364 - rel 0.035840
Error sums, total 0.335314, BP 0.107024, H 0.853966E-02, Comp 0.219750
- Maximum Relative Errors -
* BP -0.022643 at tray 7 * H 0.001972 at tray 4
Tray Glob Mat Bal 0.037533 at tray 7 * Tray Part Mat Bal 0.007331 for comp 12 at tray 6
Coln Part Mat Bal 0.002117 for comp 14

- at iter 8, err sum 0.299428, max err sum 0.598154E-01 - adj. factor 1.000000
DK/K - max .85208E-03 - min .59484E-10 - avg 0.000076
DT max - abs 4.2151 - rel 0.006603 DR max - abs 68.6970 - rel 0.034846
Error sums, total 0.299428, BP 0.993950E-01, H 0.108541E-01, Comp 0.189179
- Maximum Relative Errors -
* BP -0.022434 at tray 7 * H 0.002394 at tray 12
Tray Glob Mat Bal 0.034988 at tray 8 * Tray Part Mat Bal 0.007868 for comp 14 at tray 9
Coln Part Mat Bal 0.001112 for comp 14

- at iter 9, err sum 0.223090, max err sum 0.451418E-01 - adj. factor 1.000000
DK/K - max .69859E-03 - min .52557E-10 - avg 0.000062
DT max - abs 3.4988 - rel 0.005511 DR max - abs 60.6441 - rel 0.031253
Error sums, total 0.223090, BP 0.760023E-01, H 0.920037E-02, Comp 0.137887
- Maximum Relative Errors -
* BP -0.017252 at tray 8 * H -0.001473 at tray 9
Tray Glob Mat Bal 0.026417 at tray 8 * Tray Part Mat Bal 0.008658 for comp 14 at tray 9
Coln Part Mat Bal 0.000512 for comp 14

- at iter 10, err sum 0.120888, max err sum 0.234689E-01 - adj. factor 1.000000
DK/K - max .13657E-02 - min .96916E-10 - avg 0.000101
DT max - abs 1.9824 - rel 0.003093 DR max - abs 33.9996 - rel 0.018347
Error sums, total 0.120888, BP 0.422567E-01, H 0.394430E-02, Comp 0.746868E-01
- Maximum Relative Errors -
* BP -0.008877 at tray 8 * H -0.000723 at tray 9
Tray Glob Mat Bal 0.013870 at tray 9 * Tray Part Mat Bal 0.005120 for comp 14 at tray 9
Coln Part Mat Bal 0.000231 for comp 14

- at iter 11, err sum 0.391960E-01, max err sum 0.927780E-02 - adj. factor 1.000000
DK/K - max .10336E-02 - min .72905E-10 - avg 0.000077
DT max - abs 1.4576 - rel 0.002255 DR max - abs 26.9624 - rel 0.014341
Error sums, total 0.391960E-01, BP 0.132582E-01, H 0.434539E-02, Comp 0.215925E-01
- Maximum Relative Errors -
* BP -0.003027 at tray 9 * H 0.001915 at tray 13
Tray Glob Mat Bal 0.004336 at tray 9 * Tray Part Mat Bal 0.001514 for comp 14 at tray 10
Coln Part Mat Bal 0.000008 for comp 14

- at iter 12, err sum 0.201895E-01, max err sum 0.356961E-02 - adj. factor 1.000000
DK/K - max .12054E-02 - min .33655E-10 - avg 0.000056
DT max - abs 0.2652 - rel 0.000419 DR max - abs 4.6488 - rel 0.002341
Error sums, total 0.201895E-01, BP 0.693647E-02, H 0.117962E-02, Comp 0.120734E-01
- Maximum Relative Errors -
* BP -0.001292 at tray 8 * H 0.000254 at tray 13
Tray Glob Mat Bal 0.002024 at tray 9 * Tray Part Mat Bal 0.000529 for comp 14 at tray 10
Coln Part Mat Bal 0.000029 for comp 14

- at iter 13, err sum 0.548912E-02, max err sum 0.109176E-02 - adj. factor 1.000000
DK/K - max .75528E-03 - min .23777E-10 - avg 0.000042
DT max - abs 0.1089 - rel 0.000169 DR max - abs 2.1169 - rel 0.001174
Error sums, total 0.548912E-02, BP 0.195763E-02, H 0.278313E-03, Comp 0.325318E-02
- Maximum Relative Errors -
* BP -0.000398 at tray 8 * H -0.000078 at tray 13
Tray Glob Mat Bal 0.000615 at tray 9 * Tray Part Mat Bal 0.000158 for comp 14 at tray 10
Coln Part Mat Bal 0.000001 for comp 14
*** COLUMN CALCULATION RESOLVED ***

*** FINAL COLUMN STATUS ***									
* TRAY *	TEMP	** -TOTAL	LIQ &	VAP	OUTLET- * - LIQ. & VAP.	DRAW-OFF - *	BP.ERROR	* ENT.	BAL.ERR.*
0	56.169	2302.645		0.000	1279.248	0.000	-0.000001		0.000000
1	63.293	1042.936		2302.645	0.000	0.000	-0.000006		-0.000002
2	65.366	1040.024		2322.184	0.000	0.000	-0.000014		-0.000003
3	66.724	1030.769		2319.272	0.000	0.000	-0.000029		-0.000004
4	67.965	1017.365		2310.017	0.000	0.000	-0.000058		0.000010
5	69.284	999.701		2296.613	0.000	0.000	-0.000120		0.000011
6	70.808	976.101		2278.949	0.000	0.000	-0.000220		0.000007
7	72.690	943.982		2255.349	0.000	0.000	-0.000331		0.000017
8	75.136	901.565		2223.230	0.000	0.000	-0.000398		-0.000022
9	78.328	852.188		2180.813	0.000	0.000	-0.000370		-0.000029
10	82.160	806.307		2131.436	0.000	0.000	-0.000250		-0.000011
11	86.026	773.681		2085.555	0.000	0.000	-0.000109		0.000001
12	89.187	755.160		2052.929	0.000	0.000	-0.000015		0.000019
13	91.364	747.262		2034.408	0.000	0.000	0.000009		-0.000078
14	93.503	1880.384		1953.283	0.000	0.000	0.000004		0.000013
15	118.566	1930.023		1733.732	0.000	0.000	0.000014		0.000018
16	133.358	2051.002		1783.371	0.000	0.000	-0.000002		-0.000010
17	138.939	2115.736		1904.350	0.000	0.000	0.000003		0.000018
18	140.828	2136.512		1969.084	0.000	0.000	0.000000		0.000004
19	141.555	2144.762		1989.860	0.000	0.000	-0.000001		0.000001
20	141.921	2148.721		1998.110	0.000	0.000	-0.000001		0.000000
21	142.173	2151.181		2002.069	0.000	0.000	-0.000001		0.000000
22	142.386	2153.062		2004.529	0.000	0.000	0.000000		0.000000
23	142.584	2154.680		2006.410	0.000	0.000	0.000000		0.000000
24	142.775	2156.158		2008.028	0.000	0.000	0.000000		0.000000
25	142.963	2157.552		2009.506	0.000	0.000	0.000000		0.000000
26	143.150	2158.898		2010.900	0.000	0.000	0.000000		0.000000
27	143.335	2160.228		2012.246	0.000	0.000	0.000000		0.000000
28	143.520	2161.585		2013.576	0.000	0.000	0.000000		0.000000
29	143.706	2163.048		2014.933	0.000	0.000	0.000000		0.000000
30	143.896	2164.779		2016.396	0.000	0.000	0.000000		0.000000
31	144.095	2167.119		2018.127	0.000	0.000	0.000000		0.000000
32	144.316	2170.805		2020.467	0.000	0.000	0.000000		0.000000
33	144.584	146.652		2024.153	146.652	0.000	0.000000		0.000000
* HEATERS / COOLERS *									
TRAY 0	- DUTY	-11329.767	M-KCAL						
TRAY 33	- DUTY	11216.857	M-KCAL						
* SPECIFICATIONS *									
NO	TYPE	GIVEN	VALUE	CALC	VALUE	ERROR	CONV		
1	RECOVERY RAT	0.998000		0.998011		0.000005	Y		
2	RATE RAT	0.800000		0.799999		-0.000001	Y		
Unit op	1 - 'C2		' calculated						

*** SOLUTION OBTAINED ***

... Base case results loaded on binary file 'PROB-07 ' ...

*** UNIT 1 - 'C2' - 'DISTILLATION COLUMN' ***

--- Feed Streams ---

'S1'

- Product Streams -

'S2'

'S3'

1) * OPERATING CONDITIONS *

* Tray	* Temperature	* Pressure	*** OUTLET LIQUID ***			*** OUTLET VAPOR ***		
			* -Molar Rate-	* -Weight Rate-		* -Molar Rate-	* -Weight Rate-	
	°C	bar	kmol/h	kg/h		kmol/h	kg/h	
CON	56.17	8.00	2302.6	126971.		0.0000	0.00000	
1	63.29	8.35	1042.9	58901.3		2302.6	126971.	
2	65.37	8.38	1040.0	59464.6		2322.2	129441.	
3	66.72	8.41	1030.8	59537.1		2319.3	130004.	
4	67.96	8.45	1017.4	59397.6		2310.0	130077.	
5	69.28	8.48	999.70	59111.2		2296.6	129937.	
6	70.81	8.51	976.10	58645.6		2278.9	129651.	
7	72.69	8.54	943.98	57924.5		2255.3	129186.	
8	75.14	8.57	901.57	56900.0		2223.2	128466.	
9	78.33	8.61	852.19	55720.2		2180.8	127442.	
10	82.16	8.64	806.31	54774.3		2131.4	126263.	
11	86.03	8.67	773.68	54338.9		2085.6	125317.	
12	89.19	8.70	755.16	54308.1		2052.9	124881.	
13	91.36	8.73	747.26	54525.2		2034.4	124849.	
14	93.50	8.76	1880.4	138885.		1953.3	121082.	
15	118.57	8.80	1930.0	158963.		1733.7	125944.	
16	133.36	8.83	2051.0	176755.		1783.4	146022.	
17	138.94	8.86	2115.7	185102.		1904.4	163815.	
18	140.83	8.89	2136.5	187828.		1969.1	172161.	
19	141.55	8.92	2144.8	188858.		1989.9	174887.	
20	141.92	8.96	2148.7	189318.		1998.1	175917.	
21	142.17	8.99	2151.2	189582.		2002.1	176377.	
22	142.39	9.02	2153.1	189771.		2004.5	176641.	
23	142.58	9.05	2154.7	189927.		2006.4	176830.	
24	142.78	9.08	2156.2	190066.		2008.0	176986.	
25	142.96	9.12	2157.6	190196.		2009.5	177125.	
26	143.15	9.15	2158.9	190319.		2010.9	177255.	
27	143.33	9.18	2160.2	190440.		2012.2	177378.	
28	143.52	9.21	2161.6	190564.		2013.6	177499.	
29	143.71	9.24	2163.0	190699.		2014.9	177623.	
30	143.90	9.27	2164.8	190863.		2016.4	177758.	
31	144.10	9.31	2167.1	191090.		2018.1	177922.	
32	144.32	9.34	2170.8	191460.		2020.5	178149.	
REB	144.58	9.37	146.65	12941.0		2024.2	178519.	

- HEATER/COOLERS -

1 - Condenser -11329.767 Mcal/h

2 - Reboiler 11216.857 Mcal/h

- PRODUCT STREAMS -

Stream 'S2	', LIQUID draw-off from condenser	
Flow rate, molar	1279.248 kmol/h	- weight 70539.538 kg/h
Stream 'S3	', LIQUID draw-off from reboiler	
Flow rate, molar	146.652 kmol/h	- weight 12940.954 kg/h

- FEED STREAMS -

Stream 'S1	', Feed on tray 14	
Flow rate, molar	1425.900 kmol/h	- weight 83480.486 kg/h

- REFLUX DATA -

Molar rate	1023.397 kmol/h	Weight rate	56431.528 kg/h
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Ratios with respect to OVERHEAD product(s)

Molar	0.8000	Weight	0.8000
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Ratios with respect to TOTAL FEED

Molar	0.7177	Weight	0.6760
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2) * PRODUCT STREAMS *

* Stream 'S2		' , LIQUID	draw-off from condenser				
- Temperature		56.169 °C	- Pressure		8.0000 bar		
* No	* Component	*	-Molar Rate-	-Mol Fr-	- Weight	Rate-	-Wt Fr-
1	PROPENE		52.895	0.041348		2225.819	0.031554
2	PROPANE		40.035	0.031296		1765.554	0.025029
3	ISOBUTANE		443.703	0.346847		25788.033	0.365583
4	ISOBUTENE		3.969	0.003103		222.691	0.003157
5	1-BUTENE		155.940	0.121900		8749.353	0.124035
6	1,3-BUTADIENE		2.731	0.002135		147.704	0.002094
7	BUTANE		196.760	0.153809		11435.717	0.162118
8	TRANS-2-BUTENE		181.687	0.142027		10194.103	0.144516
9	CIS-2-BUTENE		121.548	0.095015		6819.822	0.096681
10	METHANOL		64.444	0.050376		2064.777	0.029271
11	ISOPENTANE		15.001	0.011726		1082.303	0.015343
12	METHYL TERTBUTYL ETH		0.290	0.000227		25.606	0.000363
13	TERT-BUTYL ALCOHOL		0.244	0.000190		18.058	0.000256
14	TERT-AMYL ETHER		0.000	0.000000		0.000	0.000000
* TOTAL *			1279.248	1.000000		70539.538	1.000000
			kmol/h			kg/h	
* Stream 'S3		' , LIQUID	draw-off from reboiler				
- Temperature		144.584 °C	- Pressure		9.3700 bar		
* No	* Component	*	-Molar Rate-	-Mol Fr-	- Weight	Rate-	-Wt Fr-
1	PROPENE		0.000	0.000000		0.000	0.000000
2	PROPANE		0.000	0.000000		0.000	0.000000
3	ISOBUTANE		0.000	0.000000		0.000	0.000000
4	ISOBUTENE		0.000	0.000000		0.000	0.000000
5	1-BUTENE		0.000	0.000000		0.000	0.000000
6	1,3-BUTADIENE		0.000	0.000000		0.000	0.000000
7	BUTANE		0.000	0.000000		0.000	0.000000
8	TRANS-2-BUTENE		0.000	0.000000		0.000	0.000000
9	CIS-2-BUTENE		0.000	0.000000		0.000	0.000000
10	METHANOL		0.000	0.000000		0.000	0.000000
11	ISOPENTANE		0.000	0.000000		0.000	0.000000
12	METHYL TERTBUTYL ETH		145.662	0.993248		12839.944	0.992195
13	TERT-BUTYL ALCOHOL		0.006	0.000040		0.435	0.000034
14	TERT-AMYL ETHER		0.984	0.006712		100.575	0.007772
* TOTAL *			146.652	1.000000		12940.954	1.000000
			kmol/h			kg/h	

*** STREAM DATA CALCULATION AND STORING ***

Stream 'S1' pvt/thermo/trans props calculated
Stream 'S2' pvt/thermo/trans props calculated
Stream 'S3' pvt/thermo/trans props calculated

* XPSIM, Vers. 1.06 *

* Cust/User "STAFF" *

* Proj/Problem "MTBE SEPARATION" *

* ... extended Process SIMulation ... *

- SOLUTION -

- STREAM S1 -

* Job "PROB-07" *

* Date SEP 21, 2008 *

* Page 0018 *

* STREAM 'S1', feed of unit(s) 1 'C2'

- Temperature 71.10 °C - Pressure 10.3500 bar

Phase LIQUID

Molar Flow Rate kmol/h 1425.900

Weight Flow Rate kg/h 83480.486

Molar Fraction 1.000000

Weight Fraction 1.000000

Molecular Weight 58.5458

Std Liq Vol Rate m3/h 138.0367

Enthalpy Mcal/h -5246.6152

Spec. Enthalpy kcal/kg -62.848

kcal/kmol -3679.508

Spec. Entropy kcal/kg °C 1.8676

kcal/kmol °C 109.3381

Gravity at 60/60 0.604755

Reference Gas Status - Temperature 15°C - Pressure 1 atm

No	Components	Mol. Rate	TOTAL Mol. Fr	PHASE Wt. Rate	Wt. Fr.
		kmol/h		kg /h	
1	PROPENE	52.895	0.037096	2225.819	0.026663
2	PROPANE	40.035	0.028077	1765.554	0.021149
3	ISOBUTANE	443.703	0.311174	25788.036	0.308911
4	ISOBUTENE	3.969	0.002784	222.691	0.002668
5	1-BUTENE	155.941	0.109363	8749.354	0.104807
6	1,3-BUTADIENE	2.731	0.001915	147.704	0.001769
7	BUTANE	196.760	0.137990	11435.718	0.136987
8	TRANS-2-BUTENE	181.687	0.127419	10194.104	0.122114
9	CIS-2-BUTENE	121.548	0.085243	6819.824	0.081694
10	METHANOL	64.444	0.045195	2064.777	0.024734
11	ISOPENTANE	15.001	0.010520	1082.303	0.012965
12	METHYL TERTBUTYL ETH	145.952	0.102358	12865.534	0.154114
13	TERT-BUTYL ALCOHOL	0.249	0.000175	18.492	0.000222
14	TERT-AMYL ETHER	0.984	0.000690	100.575	0.001205
***	TOTAL	1425.900	1.000000	83480.486	1.000000

* XPSIM, Vers. 1.06 *

* Cust/User "STAFF" *

* Proj/Problem "MTBE SEPARATION" *

... extended Process SIMulation ...

- SOLUTION -

- STREAM S2 -

* Page 0019 *

* Job "PROB-07" *

* Date SEP 21, 2008 *

* STREAM 'S2', product of unit 1 'C2'

- Temperature 56.17 °C - Pressure 8.0000 bar

Phase LIQUID

Molar Flow Rate kmol/h 1279.248

Weight Flow Rate kg/h 70539.538

Molar Fraction 1.000000

Weight Fraction 1.000000

Molecular Weight 55.1414

Std Liq Vol Rate m3/h 120.6815

Enthalpy Mcal/h -5190.4775

Spec. Enthalpy kcal/kg -73.582

kcal/kmol -4057.441

Spec. Entropy kcal/kg °C 1.8390

kcal/kmol °C 101.4032

Gravity at 60/60 0.584495

Reference Gas Status - Temperature 15°C - Pressure 1 atm

No	Components	Mol. Rate	TOTAL Mol. Fr	PHASE Wt. Rate	Wt. Fr.
		kmol/h		kg /h	
1	PROPENE	52.895	0.041348	2225.819	0.031554
2	PROPANE	40.035	0.031296	1765.554	0.025029
3	ISOBUTANE	443.703	0.346847	25788.033	0.365583
4	ISOBUTENE	3.969	0.003103	222.691	0.003157
5	1-BUTENE	155.940	0.121900	8749.353	0.124035
6	1,3-BUTADIENE	2.731	0.002135	147.704	0.002094
7	BUTANE	196.760	0.153809	11435.717	0.162118
8	TRANS-2-BUTENE	181.687	0.142027	10194.103	0.144516
9	CIS-2-BUTENE	121.548	0.095015	6819.822	0.096681
10	METHANOL	64.444	0.050376	2064.777	0.029271
11	ISOPENTANE	15.001	0.011726	1082.303	0.015343
12	METHYL TERTBUTYL ETH	0.290	0.000227	25.606	0.000363
13	TERT-BUTYL ALCOHOL	0.244	0.000190	18.058	0.000256
14	TERT-AMYL ETHER	0.000	0.000000	0.000	0.000000
***	TOTAL	1279.248	1.000000	70539.538	1.000000

* XPSIM, Vers. 1.06 *

* Cust/User "STAFF" *

* Proj/Problem "MTBE SEPARATION" *

* ... extended Process SIMulation ... *

- SOLUTION -

- STREAM S3 -

* Page 0020 *

* Job "PROB-07" *

* Date SEP 21, 2008 *

* STREAM 'S3', product of unit 1 'C2'

- Temperature 144.58 °C

- Pressure 9.3700 bar

Phase LIQUID

Molar Flow Rate kmol/h 146.652

Weight Flow Rate kg/h 12940.954

Molar Fraction 1.000000

Weight Fraction 1.000000

Molecular Weight 88.2426

Std Liq Vol Rate m3/h 17.3552

Enthalpy Mcal/h -169.1381

Spec. Enthalpy kcal/kg -13.070

kcal/kmol -1153.328

Spec. Entropy kcal/kg °C 1.9058

kcal/kmol °C 168.1736

Gravity at 60/60 0.745634

Reference Gas Status - Temperature 15°C

- Pressure 1 atm

No	Components	----- Mol. Rate	TOTAL Mol. Fr	PHASE Wt. Rate	----- Wt. Fr.
		kmol/h		kg /h	
1	PROPENE	0.000	0.000000	0.000	0.000000
2	PROPANE	0.000	0.000000	0.000	0.000000
3	ISOBUTANE	0.000	0.000000	0.000	0.000000
4	ISOBUTENE	0.000	0.000000	0.000	0.000000
5	1-BUTENE	0.000	0.000000	0.000	0.000000
6	1,3-BUTADIENE	0.000	0.000000	0.000	0.000000
7	BUTANE	0.000	0.000000	0.000	0.000000
8	TRANS-2-BUTENE	0.000	0.000000	0.000	0.000000
9	CIS-2-BUTENE	0.000	0.000000	0.000	0.000000
10	METHANOL	0.000	0.000000	0.000	0.000000
11	ISOPENTANE	0.000	0.000000	0.000	0.000000
12	METHYL TERTBUTYL ETH	145.662	0.993248	12839.944	0.992195
13	TERT-BUTYL ALCOHOL	0.006	0.000040	0.435	0.000034
14	TERT-AMYL ETHER	0.984	0.006712	100.575	0.007772
***	TOTAL	146.652	1.000000	12940.954	1.000000

*** STREAM INDEX ***

- ALPHABETIC ORDER -	- INPUT ORDER -
Stream Page	Stream Page
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S2 19	S2 19
S3 20	S3 20

XPSIM, Steady State Process Simulation Software
Version 1.06
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